PROPOSAL	TITLE
I	Catalysis by Coordination Compounds
II	Relationship Between Homogeneous and Heterogeneous Catalysis
III	Characterization of Catalytic Materials by New Instrumental Methods
IV	Characterization of Catalytic Materials by Chemical-Physical Methods
V	Use of Synchrotron Radiation for X-ray Photo-electron Spectroscopy

1. Title:

Catalysis by Coordination Compounds

2. Description of Project:

This project will involve the exchange of information, personnel, and the implementation of joint research programs on the fundamental aspects of the activation of molecules such as nitrogen and saturated hydrocarbons by coordination compounds of transition metals.

3. Objectives:

To achieve an understanding of the factors necessary for the activation of relatively unreactive molecules such as nitrogen, and aliphatic and aromatic hydrocarbons and for catalyzing the conversion of such molecules to specific products such as hydrazine, and inorganic nitrogen compounds.

4. Description of Activities:

A. Persons presently active in research in the fields encompassed by this proposal include:

USA: Schrauzer (UCSD); Basolo (Northwestern); Collman (Stanford); Hardy (DuPont); Parshall (DuPont); Van Tamelen (Stanford); Brintzinger (Michigan); Halpern (Chicago); Paquette (Ohio State); Bulen (Kettering Institute).

USSR: Shilov (Institute of Chemical Physics, Moscow); Vol'pin (Institute of Organometallic Chemistry); Mishustin (Microbiological Institute).

B. Since research groups in each country have distinctive experience and potential contributions to the joint research area, it is recommended that initially two to three postdoctoral level scientists from laboratories in each country (especially Shilov's laboratory) spend periods of at least a year in laboratories of the other country. At the same time, one senior person (possibly several people each spending part of a year) might be exchanged between the two countries. Soviet scientists have made particularly strong contributions to the synthetic aspects of the subject, whereas US scientists have been particularly strong on the mechanistic side. Thus, each side has a distinctive contribution to make to such a joint research program, and in turn stands to gain therefrom. One senior person from each side would be designated as program coordinator, and would be responsible for selecting personnel, participating laboratories, and organizing a small annual symposium.

5. Previous US-USSR Contacts:

Contacts to date in this field have been only informal. However, extensive references in publications by workers in each country to work in the other's country reflect a considerable degree of mutual interest.

6. Time Frame:

A program can be initiated immediately for an initial period of a minimum of 3 years. During this period, there would be exchange of senior and junior personnel among laboratories in the two countries. One joint symposium should be held annually.

7. Estimated Cost:

100 K/year to cover salaries and travel of one senior and three junior scientists, some visits by others, expendable supplies and the cost of the symposium.

8. Benefits to US:

Each country has extensive research interests and distinctive expertise for which the other country can benefit with mutual strengthening of the research of each. This field is one of very great potential technological importance.

9. Benefits to USSR:

See above.

10. Possible Security or Political Considerations:

Minimal.

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1. Title:

Relationship between Homogeneous and Heterogeneous Catalysis

2. Description of Project:

Most important industrial catalytic processes are based on heterogeneous catalysts involving gas-solid interactions. The advantages of the heterogeneous over the homogeneous systems are the ease of separating the catalyst from the reactants and products, and the minimization of corrosion. Until recently heterogeneous catalysts consisted mainly of compositions having metals or metal oxides as the active components. Recently a number of examples have been reported in which heterogeneous analogs of homogeneous catalysts, e.g. transition metal complexes, have been prepared and have been shown to exhibit reaction properties similar or identical to those of the homogeneous systems. Thus it now seems appropriate to expect that heterogeneous analogs of many homogeneous catalysts can be prepared, and to project in the future the development of heterogeneous metal complex catalysts that combine the advantages of heterogeneous and homogeneous catalysts.

3. Objectives:

a. Develop techniques for preparing heterogeneous metal complex catalysts, selecting as models well characterized homogeneous systems. Two models are proposed:

(1) An olefin hydrogenation catalyst (Ru^{+2} or phosphine complexes of Rhodium)

(2) Olefin (ethylene) oxidation over Pd to acetaldehyde.

b. Investigate the behavior of these heterogeneous analogs by:

IR spectral techniques

Kinetics

Other techniques, as applicable.

c. Compare the heterogeneous and homogeneous activity

(1) Nature of catalytic intermediates

(2) Mechanism of the reaction

d. Investigate the effects of catalyst supports and the nature of interactions between supports and metal complexes.

4. Description of Activities:

a. US workers in this field:

Academic
Prof. Collman - Stanford

Prof. S. Siegel - Arkansas

Dr. P.R. Rony - Virginia Polytech

Industry
Roth et al. - Monsanto

Haag & Whitehurst - Mobil

Heineman - Mobil

Mador - National Distillers, Division of U.S.I.

b. Soviet work in this field - some presented at International Congress on Catalysis. Golodov - (paper at Int'l Congress, Palm Beach 1972).

c. Implementation Suggestions

1. Consider the two model reactions cited above.

2. Have one system studied in US (preferably olefin hydrogenation).

3. Other system studied in USSR (ethylene oxidation over Pd)

5. Previous US-USSR Contacts:

No known previous US-USSR contacts in this field.

6. Time Frame:

Could start immediately. 3 year minimum to produce useful results.

7. Estimated Costs:

One principal investigator plus two assistants in each country for each project. Estimated total cost of $200 K / year including US salaries, travel, and expendable supplies.

8. Benefits to US:

Developing heterogeneous catalysts modeled on homogeneous systems could provide substantial practical benefits to both the US and the USSR.

9. Benefits to USSR:

Same as above.

10. Possible Security or Political Considerations:

Minimal.

1. Title: -

Characterization of Catalytic Materials by New Instrumental Methods.

2. Description of Project:

There are a variety of new spectroscopic methods which have been developed which are applicable to the study of surfaces of catalysts, to molecules bound to catalysts, and of a study of the accommodation of atoms and molecules with clean surfaces. These include:

1. X-rayphoto-electron spectroscopy (ESCA)
2. Low energy electron defraction (LEED)
3. Mossbauer spectroscopy
4. Electron spin resonance (ESR)
5. Infrared spectroscopy (IR)
6. Nuclear magnetic resonance (NMR)
7. Low-angle X-ray scattering
8. Atomic and molecular scattering from surfaces using molecular beams.

It is proposed to explore the use of these newer spectroscopic methods for the study of hetergeneous catalysts and surfaces.

3. Objectives:

To explore the utility of new instrumental methods for the study of catalytic material, and to achieve some standardization of instrumental operating conditions and interpretation of results.

4. Description of [illegible]

This project would include:

A. Providing a small number of typical catalytic materials for study in both countries. Materials might include, for example:

1. Platinum-gold, or palladium-gold catalysts

2. Rare earth-zeolite catalysts

3. Organo-metallic catalysts on a variety of supports

B. Characterization of these materials by the above spectroscopic methods in a variety of laboratories, both industrial and university.

C. Coordination of measurement program from one center in the US, and one center in the USSR, for example, the NBS in the US.

D. Selective exchange of research personnel in areas of unique competence - for example :

1. USSR - Mossbauer spectroscopy

2. US - ESCA, molecular beam spectroscopy

E. Joint publication of results.

F. The following US and Soviet groups might be suitable:

1. U.S.:

ESCA - Perlman and Hudis at Brookhaven National Laboratory; Auger spectrometry - Mark at Princeton; Mossbauer - Delgass and Boudart at Stanford;

Small angle X-ray work - Mobile Research Group at Princeton; Crystal structure - Hamilton at Brookhaven and the Mobile group; Magnetic resonance work - Lunsford at Texas A & M, and Turkevich at Princeton; ESR - Hall at Gulf, Esso Research.

2. USSR:

Mossbauer - Goldanski; Electron spin resonance - Kazanski.

5. Previous US-USSR Contacts:

Informal contacts exist between the US and Soviet specialists in most of these specific fields.

6. Time Frame:

A program could be initiated immediately, and would take at least three years to produce useful results.

7. Estimated Costs:

150 K/year would be required to support the program coordinator, salaries for 3-5 postdoctoral level scientists, travel, costs of contract measurements, and expendable supplies forthe participating laboratories.

8. Benefits to US:

Although US instrumental methods are generally more advanced than those in the USSR, they have not been systematically applied to the study of catalysts. Thus most of the sophisticated measurements would have

to be made in the US. The Soviet center could assist to take the lead in providing the materials for study. A program of this sort would help broaden the use of these instruments for the study of catalysts in US industrial and university laboratories. Exposure of the Soviet scientific community to US commercial instruments offerings could broaden the market for US products in the USSR.

9. Benefits to the USSR:

Soviets will gain experience in the application of advanced US instrumental methods to the study of catalysts.

10. Possible Security or Political Considerations:

Many advanced US instruments involve the latest electronic components, design, and packaging. They also involve computer interfacing and control. This project will not present significant risk of transfer of these technologies. However, it might raise Soviet expectations concerning the relaxation of specific export restrictions.

PROPOSAL IV

Chemical Catalysis Working Group (Haensel, Lucchesi, Ha

1. Title:

Characterization of Catalytic Materials by Chemical-Physical Methods

2. Description of Project:

During the last thirty years a variety of chemical and physical methods have been proposed for the characterization of heterogeneous catalysts, in an attempt to correlate catalytic activity with atomic, molecular and crystallographic structure. Progress has been slow, however, partially due to the fact that different investigators use different samples and there has been little consistency between the work of the various laboratories. It is proposed to correlate a number of chemical-physical methods for characterizing catalytic materials with the results of spectroscopic measurements. This will be done by applying a variety of physical-chemical methods to the study of catalysts characterized spectroscopically. Diagnostic reactions would include oxidation, acid-base catalysis, and hydrogenation-dehydrogenation. Among the chemical-physical methods of catalyst characterization to be applied in conjunction with these reaction classes one might include for example: absorption-desorption measurements, pore size distribution, particle size (crystal size) determination, phase change studies (reversible and irreversible), reaction rate measurements, etc.

3. Objectives:

To provide systematic correlations of the results of chemical-physical measurements with the results of spectroscopic characterization of catalysts.

4. Description of Activities:

Groups will be designated in the US and the USSR to take the lead respectively in one of the reaction categories, i.e. a Soviet group in oxidation and a US group in a hydrogenation-deydrogenation system. Participation of US workers with the Soviet team, and Soviet scientists with the US team, and the joint publication of results is envisioned. The catalysts selected for this study would be included in the group of materials characterized by new instrumental methods. An industrial team might be appropriate for leadership in the US - UOP, Texaco, or Gulf for example.

5. Previous US - USSR Contacts:

Regular but informal contacts exist through a joint US-Soviet participation in international symposia.

6. Time Frame:

This program must be coordinated with the project on instrumental methods. It could begin 6 months to 1 year after the instrumental measurements begin, and would require a minimum of 3 years.

7. Estimated Costs:

150 K to cover salaries of one senior and three junior scientists, travel, and expendable supplies.

8. Benefits to US:

Standardized chemical physical methods for the study of catalyst systems which are correlated with the results of spectroscopic

measurements could make an important contribution to the advance of our understanding of these systems.

9. Benefits to USSR:

Same as above.

10. Possible Security of Political Considerations:

Minimal.

1. Title:

Use of Synchrotron Radiation for X-ray Photo-electron Spectroscopy.

2. Description of Project:

The intense, broad band synchrotron radiation available from high energy accelerators or storage rings can provide a very intense source of radiation for x-ray photoelectron spectroscopy. This should allow ESCA measurements for the study of catalysts with improved sensitivity, resolution, or short response time. It should be possible to test at significantly reduced cost whether these improvements can be achieved by making joint use of US and Soviet facilities. For example, a US high-resolution electron energy spectrometer and data analysis system could be combined with a Soviet synchrotron radiation source and x-ray monochrometer.

3. Objectives:

To determine whether major improvements in sensitivity, resolution, or response time of x-ray photoelectron spectroscopic measurements on catalytic materials are possible using synchrotron radiation as the x-ray source.

4. Description of Project:

A joint US-Soviet design team would study the feasibility of combining US and Soviet components. If the combination appeared to be feasible, the necessary components would be fabricated in each country, and integrated for a series of measurements with catalystic materials. Suitable experienced design groups are available at Harvard, Wisconsin and Stanford.

5. Problems for Release:

Minimal.

6. Time Frame:

A preliminary design effort would require 1 year. Subsequent equipment fabrication and joint experiments would require 3 additional years.

7. Estimated Costs:

$100 K to support US design team of 3 people for 1 year, including travel for 3 or 4 meetings of joint design team.

8. Benefits to US:

This project would enable us to explore new instrumental methods at reduced costs.

9. Benefits to USSR:

See above.

10. Possible Security or Political Considerations:

Minimal.

ROUTING AND RECORD SHEET

SUBJECT: (Optional)

PROPOSALS ON CHEMICAL CATALYSIS FOR US-SOVIET EXCHANGE PROGRAM

FROM: [redacted]
East-West Exchanges Staff/SBD/DCS
902 Key

EXTENSION: 2492

NO.

DATE: 18 Aug 72

TO: (Officer designation, room number, and building)	DATE RECEIVED	DATE FORWARDED	OFFICER'S INITIALS	COMMENTS (Number each comment to show from whom to whom. Draw a line across column after each comment.)
1. [redacted] OSI 6F 36	18 Aug		[redacted]	Per [redacted] telecon this date STATINTL We are forwarding this to you for your comments. May we have ~~your comments~~ them as soon as possible. As this is our only ~~comments~~ copy; we would appreciate your returning to us upon completion. Thank you. [redacted] STATINTL
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